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FILE COVERS 1907 - 24 Dec 2003 VOL 139 ISS 26  
FILE LAST UPDATED: 23 Dec 2003 (20031223/ED)

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=> s (paral?(w) mass (w)spectr?)
      321747 PARAL?
      788655 MASS
      71248 MASSES
      826335 MASS
          (MASS OR MASSES)
      2285432 SPECTR?
L10      16 (PARAL?(W) MASS (W)SPECTR?)
```

=> d bib,abs 1-16

```
L10 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:289440 CAPLUS
DN 139:193345
TI A generic assay for phosphate-consuming or -releasing enzymes coupled
on-line to liquid chromatography for lead finding in natural products
AU Schenk, T.; Appels, N. M. G. M.; van Elswijk, D. A.; Irth, H.; Tjaden, U.
R.; van der Greef, J.
CS Kiadis B.V., Leiden, 2333 CA, Neth.
SO Analytical Biochemistry (2003), 316(1), 118-126
CODEN: ANBCA2; ISSN: 0003-2697
PB Elsevier Science
DT Journal
LA English
AB A generic continuous-flow assay for phosphate-consuming or -releasing
enzymes coupled online to liq. chromatog. (LC) has been developed.
Operating the LC-biochem. assay in combination with mass spectrometry
allows the fast detection and identification of inhibitors of these
enzymes in complex mixts. The assay is based on the detection of
phosphate, released by the online continuous-flow enzymic reaction, using
a fluorescent probe. The probe consists of fluorophore-labeled
phosphate-binding protein, which shows a strong fluorescence enhancement
upon binding to inorg. phosphate. To detect very small changes of the
phosphate concn. in a postcolumn enzymic reaction medium, the enzymic
removal of phosphate impurities from solvents, reagents, and samples was
optimized for application in continuous flow. The potential of the
```

phosphate probe is demonstrated by monitoring the enzymic activity, i.e., the phosphate release, from alk. phosphatase. The selectivity of the phosphate readout, necessary to distinguish between phosphate contg. substrate or product and free inorg. phosphate released after enzymic conversion, is shown. The applicability of LC coupled to the enzymic assay using the phosphate readout was demonstrated by detection of tetramisole in a plant ext. as inhibitor of alk. phosphatase.

**Parallel mass spectrometry** allowed the simultaneous confirmation of the identity of the inhibitor.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:949675 CAPLUS  
DN 139:134016  
TI TEM Imaging of Mass-selected Polymer Molecules  
AU Nasibulin, Albert G.; Kauppinen, Esko I.; Thomson, Bruce A.; Fernandez de la Mora, J.  
CS Aerosol Technology Group, VTT Processes, FIN-02044, Finland  
SO Journal of Nanoparticle Research (2002), 4(5), 449-453  
CODEN: JNARFA; ISSN: 1388-0764  
PB Kluwer Academic Publishers  
DT Journal  
LA English  
AB Polyethylene glycol (PEG) mols. with masses below 1300 amu are electrosprayed (ES) from soln., mobility-selected at high resolu. in a differential mobility analyzer (DMA), collected on a grid and imaged by transmission electron microscopy (ES-DMA-TEM). The DMA resolves individual n-mers, and selects only one out of the many present in the original sample. Ion identity is established from **parallel mass spectra** (ES-MS). The images reveal spherical particles 1.46 nm in diam., in good agreement with the known ion mass and bulk d. The DMA-selection technique opens new paths for the study of very small particles.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 2002:688793 CAPLUS  
DN 137:358560  
TI Thermal Stability of Self-Assembled Monolayers: Influence of Lateral Hydrogen Bonding  
AU Valiokas, Ramunas; Oestblom, Mattias; Svedhem, Sofia; Svensson, Stefan C. T.; Liedberg, Bo  
CS Division of Applied Physics, Division of Chemistry, Department of Physics and Measurement Technology, Linköping University, Linköping, S-581 83, Swed.  
SO Journal of Physical Chemistry B (2002), 106(40), 10401-10409  
CODEN: JPCBFK; ISSN: 1520-6106  
PB American Chemical Society  
DT Journal  
LA English  
AB Temp.-programmed desorption (TPD) of self-assembled monolayers (SAMs) on Au is studied by using in **parallel mass spectrometry** (MS) and IR reflection-absorption spectroscopy (IRAS). Monolayers formed by HS(CH<sub>2</sub>)<sub>n</sub>-OH (n = 18, 22) and HS(CH<sub>2</sub>)<sub>15</sub>-CONH-(CH<sub>2</sub>CH<sub>2</sub>O)-H (EG1) are compared to reveal the influence of specifically introduced hydrogen-bonding groups on their thermal stability. The overall desorption process of the above mols. occurs in 2 main steps; a disordering of the alkyl chains followed by a complex series of decompn./desorption reactions. The final step of the process involves desorption of S from different chemisorption states. The amide-group-contg. SAM, which is stabilized by lateral hydrogen bonds, displays a substantial delay of the alkyl chain disordering by .apprx.50

K, as compared to the linear chain alcs. HS(CH<sub>2</sub>)<sub>n</sub>-OH. also, the decompn. of the alkyls and the onset of S desorption occur at a temp. that is higher by .apprx.25 K as compared to the HS(CH<sub>2</sub>)<sub>18</sub>-OH SAM. The desorption process is also studied for 2 oligo(ethylene glycol)-terminated SAMs, HS(CH<sub>2</sub>)<sub>15</sub>-X-(CH<sub>2</sub>CH<sub>2</sub>O)<sub>4</sub>-H (EG<sub>4</sub>-SAMs), where X is -CONH- and -COO- linking groups. In addn. to the mol. chain disordering, the decompn./desorption process of the EG<sub>4</sub>-SAMs occurs in 2 steps. The 1st is assocd. with the loss of the oligomer portion and the 2nd with the desorption of the alkylthiolate part of the mol. Study points out that lateral hydrogen bonding, introduced via amide groups, is a convenient way to improve the thermal stability of alkanthiolate SAMs.

RE.CNT 52        THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD  
                 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10    ANSWER 4 OF 16    CAPLUS    COPYRIGHT 2003 ACS on STN

AN    2002:59880    CAPLUS

DN    136:262794

TI    Neutral products from gas phase rearrangements of simple carbocations

AU    Morton, Thomas Hellman

CS    Department of Chemistry, University of California, Riverside, CA,  
      92521-0403, USA

SO    Advances in Gas Phase Ion Chemistry (2001), 4, 213-256

      CODEN: AGPCER; ISSN: 1071-9687

PB    JAI Press Inc.

DT    Journal; General Review

LA    English

AB    A review; analyzing the neutral products from ionic reactions in the gas phase provides information that cannot be gained by mass spectrometric methods alone. Neutrals have been recovered using three general techniques for generating ions in sufficient quantities: nuclear decay of multiply tritiated precursors, .gamma.-radiolysis studies, and electron bombardment flow (EBFlow) expts. Analyses of the uncharged reaction products of ion-mol. reactions are most effectively interpreted in conjunction with **parallel mass spectrometric** investigations. Taken together, these combined studies demonstrate the propensity of gaseous cations to undergo similar sorts of isomerizations as have been reported in condensed media. The absence of solvent and counterions makes it possible to produce ions in the gas phase that cannot be formed in soln. Despite the difference in reaction medium, the same two general categories of rearrangement-ring closure/ring opening and atom/group transfer-account for the variety of ion structures that give rise to the obsd. neutral products.

RE.CNT 95        THERE ARE 95 CITED REFERENCES AVAILABLE FOR THIS RECORD  
                 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10    ANSWER 5 OF 16    CAPLUS    COPYRIGHT 2003 ACS on STN

AN    2000:106149    CAPLUS

DN    133:101503

TI    A multiple electrospray interface for **parallel mass spectrometric** analyses of compound libraries

AU    Wang, T.; Zeng, L.; Cohen, J.; Kassel, Daniel B.

CS    CombiChem, Inc., San Diego, CA, USA

SO    Combinatorial Chemistry and High Throughput Screening (1999), 2(6),  
      327-334

      CODEN: CCHSFU; ISSN: 1386-2073

PB    Bentham Science Publishers

DT    Journal

LA    English

AB    A parallel spray interface for mass spectrometry is described. This new electrospray interface enables effluent flow streams from an array of HPLC columns to be sampled independently and sequentially on a chromatog. time-scale. Unlike our previously reported parallel LC-MS interface, which incorporated a dual-sheath spray interface accommodating up to four flow streams that are sampled simultaneously, this new interface permits

up to four columns to be sampled sequentially by means of a stepping motor and rotating plate assembly. Effluent flow streams from an array of four HPLC columns are connected to a parallel arrangement of electrospray needles co-axial to the mass spectrometer entrance aperture. Within the needle assembly, the individual spray tips are oriented in a circular array, where each needle is situated 90 degrees relative to one another for four-column operation. An eight-column system is described with needles spaced at 45 degree intervals. In between the needle assembly and the mass spectrometer entrance aperture is a Teflon disk with a through-hole that is mounted to a stepping motor assembly. By precisely controlling the stepping of the motor assembly, it is possible to "sample" each of the spray positions multiple times per s. By operating the quadrupole mass spectrometer in the single ion monitoring (SIM) mode, it was possible to acquire data at each of the spray positions during the course of the elution of compds. from the HPLC column array while maintaining both good sensitivity and peak shape. Preliminary results suggest this technique will be useful for high throughput combinatorial library anal. and profiling.

RE.CNT 17      THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1998:148610 CAPLUS

DN 128:267854

TI Dual **parallel mass spectrometers** for  
analysis of sphingolipid, glycerophospholipid and plasmalogen molecular  
species

AU Byrdwell, Wm. Craig

CS FQS, NCAUR, ARS, USDA, Peoria, IL, 61604, USA

SO Rapid Communications in Mass Spectrometry (1998), 12(5), 256-272

CODEN: RCMSEF; ISSN: 0951-4198

PB John Wiley & Sons Ltd.

DT Journal

LA English

AB Anal. of phospholipids was performed using a liq. chromatog. sepn. with two mass spectrometers in parallel providing electrospray ionization (ESI) and atm. pressure chem. ionization (APCI) data simultaneously from a triple quadrupole instrument and a single quadrupole instrument, resp. The output from UV-Vis and evaporative light scattering detectors were also acquired by the two mass spectrometers, resp., for four detectors overall. This arrangement was used to identify and calc. area percents for mol. species of dihydrosphingomyelin (DHS) and sphingomyelin (SPM) in com. available bovine brain SPM, in human plasma ext. and in porcine lens ext. Mol. species of phosphatidylethanolamine and its plasmalogen, and phosphatidylcholine and its plasmalogen were identified and semi-quant. anal. performed. Com. available bovine brain SPM was found to contain 11.5% DHS and 88.5% SPM. The only DHS mol. species identified in human plasma was 16:0-DHS, at or below 1% of the sphingolipid content. Porcine lens membranes were found to contain 14.4% DHS and 85.6% SPM. Other findings reported here include: (1) phospholipids were found to undergo dimerization in the electrospray source, giving masses representing combinations of species present. (2) Triacylglycerols gave usable mass spectra under electrospray ionization conditions, as well as under APCI-MS conditions. (3) Triacylglycerols gave ammonium adducts as base peaks in their APCI mass spectra, which reduced fragmentation and increased the proportions of mol. ions. (4) Mass spectra were obtained for phospholipids which underwent both protonation and sodium adduct formation in different chromatog. runs. This paper was prepd. under the auspices of the US Government and it is therefore not subject to copyright in the US.

RE.CNT 26      THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1998:45137 CAPLUS

DN 128:75016  
TI Methanol Oxidation on Rhodium As Probed by Surface-Enhanced Raman and Mass Spectroscopies: Adsorbate Stability, Reactivity, and Catalytic Relevance  
AU Williams, Christopher T.; Takoudis, Christos G.; Weaver, Michael J.  
CS School of Chemical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN, 47907, USA  
SO Journal of Physical Chemistry B (1998), 102(2), 406-416  
CODEN: JPCBFK; ISSN: 1089-5647  
PB American Chemical Society  
DT Journal  
LA English

AB The relationship between surface speciation and catalytic activity/selectivity during methanol oxidn. on polycryst. rhodium under ambient-pressure flow-reactor conditions was studied from 25 to 500 .degree.C by means of surface-enhanced Raman spectroscopy (SERS) along with **parallel mass spectrometric** (MS) measurements. By utilizing SERS-active Rh films formed by electrodeposition onto gold, the former technique provides in situ surface vibrational spectra with unique sensitivity under these demanding conditions, enabling adsorbed species to be probed in real time (.apprxeq.1 s) for comparison with the overall kinetics as evaluated by MS. Exposure of Rh to O2-free methanol yielded no detectable vibrational bands between 25 and 500.degree., although methanol decompn. to form CO and H2 was evident from MS. The presence of even subunity molar ratios of oxygen, however, yielded rich SER spectra, highlighted by bands indicative of CO(ads) (.nu.Rh-CO = 465 cm-1, .nu.Rh-CO = 2000 cm-1). The catalytic selectivity toward CO2 (vs. CO) gaseous product formation decreased markedly around the desorption temp. of CO(ads) .apprxeq. 350.degree. under these conditions. This is consistent with the facilitation of CO2 prodn. by the presence of CO(ads). Complete selectivity toward exhaustive methanol oxidn. (i.e., CO2, H2O formation) was obsd. in oxygen-rich methanol mixts., adsorbed CO now being absent at all temps. The CO2 prodn. occurs partly via methanolic C-O cleavage as deduced by 18O2 substitution. The presence of rhodium oxide (Rh2O3) was diagnosed with such reactant mixts. above ca. 300 .degree.C from the characteristic 500-580 cm-1 .nu.Rh-O bands. The kinetics of formation and removal of the oxide were probed by gas flow switching coupled with transient SERS measurements. The oxide formation rates following O2 exposure are slowed markedly (>100-fold) by the presence of even a small (5%) methanol mole fraction. Switching to pure methanol results in very rapid oxide redn., so that, for example, removal is complete within ca. 1s at 350.degree. with 100 Torr of CH3OH. Examm. of the transient oxide removal kinetics as a function of temp. and methanol pressure revealed a transition from strongly activated to essentially T-independent behavior at lower pressures and/or higher temps. This is indicative of a change from rate-detg. removal of oxygen from the oxide lattice to a subsequent step involving formation of and/or reaction with an adsorbed methanol scavenger. While such reactivity earmarks the oxide as a potential reaction intermediate, the overall catalytic turnover rates for methanol oxidn. are nonetheless faster than can be accommodated on this basis.

RE.CNT 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1997:410724 CAPLUS  
DN 127:155996  
TI Probing Combinatorial Library Diversity by Mass Spectrometry  
AU Demirev, Plamen A.; Zubarev, Roman A.  
CS Division of Ion Physics The Aangstroem Laboratory, Uppsala University, Uppsala, S-751 21, Swed.  
SO Analytical Chemistry (1997), 69(15), 2893-2900  
CODEN: ANCHAM; ISSN: 0003-2700  
PB American Chemical Society  
DT Journal

LA English  
AB The feasibility of a massively **parallel mass spectrometric** method for probing combinatorial library diversity is addressed theor. for the example of computer-generated mass distributions of combinatorially synthesized peptide libraries contg. between two and seven amino acids. The authors study the behavior of several global (integral) parameters of such mass distributions-mass centroid, dispersion, skewness, and kurtosis. The centroid and dispersion carry information that may characterize the completeness of the synthetic effort. Local mass distribution parameters, e.g., mass d. (no. of peptides per mass interval), are also examd. The practical implementation and eventual limitations of such an approach are discussed as well.

L10 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1996:667782 CAPLUS

DN 125:320017

TI Detection of the picolinic acid biomarker in Bacillus spores using a potentially field-portable pyrolysis-gas chromatography-ion mobility spectrometry system

AU Snyder, A. Peter; Thornton, Sidney N.; Dworzanski, Jacek P.; Meuzelaar, Henk L. C.

CS Dev. Eng. Cent., U.S. Army Edgewood Res., Aberdeen Proving Ground, MD, 21010-5423, USA

SO Field Analytical Chemistry and Technology (1996), 1(1), 49-59

CODEN: FACTFR; ISSN: 1086-900X

PB Wiley

DT Journal

LA English

AB The absence of a field-portable device to provide real-time detection of Gram-pos. bacterial spores has prompted the interfacing of a pyrolysis (Py) module to an existing, hand-held gas-chromatog.-ion-mobility spectrometry (GC/IMS) device. In this configuration, spore detection is achieved by the observation of picolinic acid (PA), which is the most characteristic pyrolysis decompn. product of the parent dipicolinic (2,6-pyridinedicarboxylic) acid (DPA). Pos. identification of PA was demonstrated using a lab.-based GC instrument with dual, **parallel mass spectrometry** (MS) and IMS detectors. Spores and vegetative microorganisms of the genus Bacillus were characterized by the presence and absence of DPA, resp., and the picolinic acid marker was identified from the GC/IMS and GC/MS profiles. A field-portable prototype Py-GC/IMS system is described and appears to provide similar bioanal. information with respect to the lab.-based system. Preliminary results of this study indicate that the degree of compd. sepn. afforded by a short GC capillary column guards against common environmental interferences including urban particulate matter and biol. particles such as fungal spores and pollen.

L10 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1987:429781 CAPLUS

DN 107:29781

TI Determination of the nuclear reactor burning process balance by gamma spectrometry of fission products. Part V - Determination of the isotopic composition of irradiated uranium

AU Bulovic, V.; Maksimovic, Z.; Krtic, J.; Sus, F.; Klosova, E.

CS Boris Kidric Inst. Nucl. Sci., Vinca, Yugoslavia

SO Jaderna Energie (1987), 33(1), 8-11

CODEN: JADEAQ; ISSN: 0448-116X

DT Journal

LA English

AB The possibility of detg. the isotopic compn. of irradiated U fuel of a heavy water reactor on the basis of .gamma.-spectrometry of fission products was exptl. tested. The testing was performed upon spent fuel from unenriched U. For detg. the fission products (106Ru, 134Cs and 137Cs) a spectrometer with a Ge(Li) detector was used. The accuracy of

the results obtained for the compn. of U was tested through its **parallel mass-spectrometric** analyses.

L10 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1987:112632 CAPLUS  
DN 106:112632  
TI The thermal decomposition of strontium fluorophosphate hydrate  
( $\text{SrPO}_3\text{F} \cdot \text{H}_2\text{O}$ )  
AU Menz, D. H.; Heide, K.; Kunert, C.; Mensing, C.; Kolditz, L.  
CS Zentralinst. Anorg. Chem., Dtsch. Akad. Wiss., Berlin, DDR-1199, Ger. Dem.  
Rep.  
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1986), 540-541, 191-7  
CODEN: ZAACAB; ISSN: 0044-2313  
DT Journal  
LA German  
AB The thermal decompn. of  $\text{SrPO}_3\text{F} \cdot \text{H}_2\text{O}$  was studied by complex thermal anal.  
The thermogravimetric study was completed by simultaneous and  
**parallel mass spectrometric** anal. of the gas  
phase. During the 1st state of thermal decompn. .apprx.0.8 mol water is  
lost. Then a partial hydrolysis takes place and HF is formed. The  
formation of  $\text{POF}_3$  is a multistage mechanism without effect of  $\text{H}_2\text{O}$  at  
>500.degree.. The partial reactions leading to .alpha.- $\text{Sr}_2\text{P}_2\text{O}_7$  and  $\text{SrF}_2$   
>600.degree. and to .alpha.- $\text{Sr}_2\text{P}_2\text{O}_7$  and  $\text{Sr}_5(\text{PO}_4)_3\text{F}$  >750.degree. were  
formulated and the exptl. and calcd. mass loss were compared.

L10 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1985:196916 CAPLUS  
DN 102:196916  
TI Thermal decomposition of calcium phosphorofluoridate dihydrate  
( $\text{CaPO}_3\text{F} \cdot 2\text{H}_2\text{O}$ )  
AU Heide, K.; Menz, D. H.; Schmidt, C.; Kolditz, L.  
CS Sekt. Chem., Friedrich-Schiller-Univ., Jena, DDR-6900, Ger. Dem. Rep.  
SO Zeitschrift fuer Anorganische und Allgemeine Chemie (1985), 520, 32-8  
CODEN: ZAACAB; ISSN: 0044-2313  
DT Journal  
LA German  
AB The thermal decompn. of  $\text{CaPO}_3\text{F} \cdot 2\text{H}_2\text{O}$  was studied by thermogravimetry under  
inert conditions. A **parallel mass  
spectrometric** anal. of gases produced was made. With the use of  
an effusion cell a quasiequil. evapn. in the vicinity of the ion source of  
the spectrometer was achieved. The results are comparable with the  
thermogravimetric anal. under normal pressure. During 1st stage of  
thermal decompn. 1 mol  $\text{H}_2\text{O}$  was lost. The further course is detd. by  
release of HF and  $\text{POF}_3$ . The several steps of decompn. leading to  
.alpha.- $\text{Ca}_2\text{P}_2\text{O}_7$  at >360.degree. are discussed.

L10 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1985:178482 CAPLUS  
DN 102:178482  
TI Method and apparatus for **parallel mass  
spectrometry**  
PA Chang, Chuang, USA  
SO Jpn. Kokai Tokkyo Koho, 16 pp.  
CODEN: JKXXAF  
DT Patent  
LA Japanese  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59176663	A2	19841006	JP 1984-41208	19840303
	US 4507555	A	19850326	US 1983-472161	19830304
PRAI	US 1983-472161		19830304		
AB	The design is claimed of a <b>parallel mass spectrometric</b> app. joined in tandem with a gas chromatograph.				

L10 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1985:159764 CAPLUS  
DN 102:159764  
TI **Parallel mass spectrometry** for high  
performance GC and LC detection  
AU Chang, C.  
CS Wright State Univ., Dayton, OH, USA  
SO American Laboratory (Shelton, CT, United States) (1985), 17(3), 59-64, 66  
CODEN: ALBYBL; ISSN: 0044-7749  
DT Journal; General Review  
LA English  
AB A review with 15 refs. Problem areas in using conventional scanning mass spectrometers for high-performance gas chromatog. (GC) and liq. chromatog. (LC) detection are discussed. The potential use of **parallel mass spectrometers** to avoid these problems is also discussed.

L10 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1976:600351 CAPLUS  
DN 85:200351  
TI Valence level photoelectron spectra of some heavy group 4-6 diatomic molecules  
AU Wu, M.; Fehlner, T. P.  
CS Dep. Chem., Univ. Notre Dame, Notre Dame, IN, USA  
SO Journal of the American Chemical Society (1976), 98(24), 7578-85  
CODEN: JACSAT; ISSN: 0002-7863  
DT Journal  
LA English  
AB The He I photoelectron spectra of GeS, GeSe, SnS, SnTe, and PbTe in the gas phase were obtained by the photoionization of the vapors above appropriate solids at 700-1000.degree.K. Spectra are assigned by using obsd. relative band areas, vibrational fine structure, and spin-orbit splitting along with electron impact ionization potentials and **parallel mass spectrometric studies**. There is significant mixing of the .SIGMA.1/2 and .PI.1/2 states in the heavier species. Distinct differences between the .PI. states of light and heavy diatomics are obsd. Similarities and differences between the valence regions of group 4-6 diatomics and diatomics of group 5-5 and group 3-7 are also reported.

L10 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN  
AN 1959:15979 CAPLUS  
DN 53:15979  
OREF 53:2923h-i,2924a  
TI Anomalous behavior of gem-diethers in the mass spectrometer  
AU LeBlanc, R. Bruce  
CS Dow Chem. Co., Freeport, TX  
SO Anal. Chem. (1958), 30, 1797-9  
CODEN: ANCHAM; ISSN: 0003-2700  
DT Journal  
LA Unavailable  
AB gem-Diether (compds. with 2 alkoxy groups on the same C atom) were measured in the mass spectrometer. They give different spectra, depending on whether the filament is bare W or carbonized W. The carbonized filament gives the normal spectrum. The bare filament causes a partial decompn. into a vinyl ether and alc. For example, MeCH(OEt)2 on decompn. yields EtOH and CH2:CHOEt. For reliable analysis of the compds. a carbonized filament is recommended.



(FILE 'WPIDS' ENTERED AT 16:18:38 ON 24 DEC 2003)

FILE 'USPATFULL' ENTERED AT 16:21:50 ON 24 DEC 2003

L4 1 S (PARALLEL(W) MASS (W) SPECTROMETRY)/TI,AB,CLM  
L5 2 S (PARALLEL(W) MASS (W) SPECTROMETRY)/TI,AB,CLM  
L6 3 S (PARALLEL(W) MASS (W) SPECTR?)/CLM,AB,TI  
L7 3 S (PARAL?(W) MASS (W) SPECTR?)/CLM,AB,TI  
L8 9 S (PARAL?(W) MASS (W) SPECTR?)  
L9 8 S L8 AND PROTEIN

=> d bib,kwic 1-8

L9 ANSWER 1 OF 8 USPATFULL on STN  
AN 2003:173349 USPATFULL  
TI System and method for high throughput screening of droplets  
IN Hess, Robert, Arlington, MA, UNITED STATES  
Brenan, Colin, Marblehead, MA, UNITED STATES  
Linton, John, Lincoln, MA, UNITED STATES  
Ozbal, Can, Cambridge, MA, UNITED STATES  
Green, Donald, Watertown, MA, UNITED STATES  
Hunter, Ian, Lincoln, MA, UNITED STATES  
PI US 2003119193 A1 20030626  
AI US 2002-267912 A1 20021008 (10)  
RLI Continuation-in-part of Ser. No. US 2001-842361, filed on 25 Apr 2001,  
PENDING  
DT Utility  
FS APPLICATION  
LREP BROMBERG & SUNSTEIN LLP, 125 SUMMER STREET, BOSTON, MA, 02110-1618  
CLMN Number of Claims: 90  
ECL Exemplary Claim: 1  
DRWN 14 Drawing Page(s)  
LN.CNT 2283  
CAS INDEXING IS AVAILABLE FOR THIS PATENT.  
SUMM . . . speeds at which large numbers of samples can be analyzed.  
Unlike optical-based assays in which samples can be analyzed in  
**parallel, mass spectrometry** is a serial  
process in which sample must be analyzed one-at-a-time. Typically, a  
slow desalting step or purification step is. . .  
SUMM . . . seconds. In various embodiments, the rate is substantially one  
assay per second. The reaction may also be buffered only by  
**proteins** intrinsic to the assay such as the enzyme in an enzyme  
inhibition assay.  
DETD [0121] .alpha.-Chymotrypsin is a protease that cleaves **proteins**  
and peptides at aromatic amino acids such as phenylalanine, tyrosine,  
and tryptophan. The example assay attempts to discover inhibitors of. .

L9 ANSWER 2 OF 8 USPATFULL on STN  
AN 2002:268969 USPATFULL  
TI Mass spectrometer apparatus for analyzing multiple fluid samples  
concurrently  
IN Moini, Mehdi, Austin, TX, United States  
Jiang, Longfei, Austin, TX, United States  
PA Board of Regents, The University of Texas System, Austin, TX, United  
States (U.S. corporation)  
PI US 6465776 B1 20021015  
AI US 2000-586588 20000602 (9)  
DT Utility  
FS GRANTED  
EXNAM Primary Examiner: Lee, John R.; Assistant Examiner: Vanore, David A.  
LREP Fulbright & Jaworski, LLP  
CLMN Number of Claims: 24  
ECL Exemplary Claim: 1

DRWN 2 Drawing Figure(s); 2 Drawing Page(s)

LN.CNT 713

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM . . . of dual ESI sprayers have been tried with a Y-shaped orifice defined within the nozzle in order to investigate electrosprayed **proteins** using ion-ion or ion-molecule reactions. In particular the accurate measurement of masses of organic compounds has been another use of. . .

SUMM . . . Corporation on a "Hot Gas Sampling"; and U.S. Pat. No. 4,507,555 patented Mar. 26, 1985 to C. Chang on a "**Parallel Mass Spectrometer**"; and U.S. Pat. No. 4,562,351 patented Dec. 31, 1985 to P. Atherton et al and assigned to VG Instruments Group. . .

L9 ANSWER 3 OF 8 USPATFULL on STN

AN 2002:191521 USPATFULL

TI Massive parallel method for decoding DNA and RNA

IN Ju, Jingyue, Englewood Cliffs, NJ, UNITED STATES

Li, Zengmin, New York, NY, UNITED STATES

Edwards, John Robert, New York, NY, UNITED STATES

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PI US 2002102586 A1 20020801

US 6664079 B2 20031216

AI US 2001-972364 A1 20011005 (9)

RLI Continuation-in-part of Ser. No. US 2000-684670, filed on 6 Oct 2000, PENDING

PRAI US 2001-300894P 20010626 (60)

DT Utility

FS APPLICATION

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CLMN Number of Claims: 60

ECL Exemplary Claim: 1

DRWN 28 Drawing Page(s)

LN.CNT 1869

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM [0034] The invention provides a **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .

DRWD [0057] FIG. 24: **Parallel mass spectrometry** system for DNA sequencing. Example shows three mass spectrometers in parallel. Samples are injected into the ion source where they. . .

DETD . . . In one embodiment, the mass tag is a 2-nitro-.alpha.-methyl-3,4-dimethoxybenzyl group. In one embodiment, the mass tag is detected using a **parallel mass spectrometry** system which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .

DETD [0133] The invention provides a **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .

DETD . . . areas of biomedical research. Though these ionization methods are suitable for the analysis of bioorganic molecules, such as peptides and **proteins**, improvements in both detection and sample preparation are required for implementation of mass spectrometry for DNA sequencing applications. Since the. . .

DETD [0151] The photocleavable 2-nitrobenzyl moiety has been used to link biotin to DNA and **protein** for efficient removal by UV light (.about.350 nm) (Olejnik et al. 1995, 1999). In the approach disclosed herein the 2-nitrobenzyl. . .

DETD . . . not capped. As discussed above, the photo cleavable 2-nitro benzyl moiety has been used to link biotin to DNA and **protein** for efficient removal by UV light (.about.350 nm) irradiation (Olejnik

et al. 1995, 1999). Four different 2-nitro benzyl groups with. . .

DETD [0172] To make mass spectrometry competitive with a 96 capillary array method for analyzing DNA, a **parallel mass spectrometer** approach is needed. Such a complete system has not been reported mainly due to the fact that most of the. . .

DETD [0173] A complete **parallel mass spectrometry** system includes multiple APCI sources interfaced with multiple analyzers, coupled with appropriate electronics and power supply configuration. A mass spectrometry. . . figures show a system with three mass spectrometers in parallel. Higher throughput is obtained using a greater number of in **parallel mass spectrometers**.

CLM What is claimed is:  
 26. The method of claim 17, wherein the mass tag is detected using a **parallel mass spectrometry** system which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. . .  
 54. A **parallel mass spectrometry** system, which comprises a plurality of atmospheric pressure chemical ionization mass spectrometers for parallel analysis of a plurality of samples. .

L9 ANSWER 4 OF 8 USPTAFULL on STN

AN 2002:133513 USPTAFULL

TI Proteomic analysis by **parallel mass spectrometry**

IN Ladine, James R., Uxbridge, MA, UNITED STATES *ap 5.*  
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Story, Mike S., Los Gatos, CA, UNITED STATES

PI US 2002068366 A1 20020606

AI US 2001-835273 A1 20010413 (9)

PRAI US 2000-196889P 20000413 (60)

DT Utility

FS APPLICATION

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CLMN Number of Claims: 28

ECL Exemplary Claim: 1

DRWN 7 Drawing Page(s)

LN.CNT 1181

TI Proteomic analysis by **parallel mass spectrometry**

SUMM [0002] This invention relates to proteomic analysis by **parallel mass spectrometry**.

SUMM [0003] Within a typical cell there are several thousand **proteins**, its "proteome," which carry out the metabolic work of the cell. These **proteins** are in constant interplay with one another, and with every other sort of biomolecule found within a cell. The **proteins** physically interact, or bind, to each other and to common secondary molecules. The result of such interactions is a fine control and balancing of metabolic functions. For example, one **protein** may increase or decrease the function of another **protein** by binding to it and altering its structure by the addition or removal of a modifying group such as a phosphate. Another mode of action is for one **protein** to produce more or less of a secondary substance that interacts allosterically with a second **protein** (or multiple second **proteins**) to modulate its function. Analysis of the abundance of **proteins** can therefore be useful in elucidating the molecular basis of differences brought about by diseases or by therapeutic treatments

SUMM [0004] A number of techniques have been suggested for analyzing cellular **proteins**, including, for example, two-dimensional electrophoresis followed by mass spectrometry. In the case of two-dimensional electrophoresis, a **protein** sample is placed in

array to a common computing device, said mass spectral data being indicative of the identity and the abundance of **protein** in said multiple sample, and correlating said mass spectral data as a function of time.

2. The method of claim 1 comprising displaying said correlated data as a function of **protein** identity, **protein** abundance, and time.

4. The method of claim 1 comprising identifying **proteins** based on changes in abundance as a function of time.

6. The method of claim 4 comprising analyzing 500 **proteins** or more.

7. The method of claim 6 comprising analyzing 5000 **proteins** or more.

22. A method for analysis of **proteins** in a biological system comprising: providing a biological system containing **proteins**; exposing the biological system to a stimulus; after exposing the biological system to the stimulus, sampling the biological system at multiple time intervals to obtain multiple samples; treating the multiple samples by a separation technique to provide multiple **protein** samples suitable for analysis by mass spectrometry; providing a parallel array of mass spectrometer systems capable of simultaneous analysis of as many **protein** samples as there are spectrometer systems in said array; analyzing the multiple **protein** samples in said parallel array of mass spectrometry systems to generate mass spectral data indicative of the identity and the abundance of **proteins** in said multiple **protein** samples; and in a common electronic computing device communicating with each of said mass spectrometry systems, correlating said mass spectral.

27. The system of claim 26 wherein the analysis includes analysis of about 500 **proteins** or more.

L9 ANSWER 5 OF 8 USPATFULL on STN

AN 1999:18911 USPATFULL

TI Methods and apparatus for sequencing polymers with a statistical certainty using mass spectrometry

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PI US 5869240 19990209

AI US 1995-447175 19950519 (8)

DT Utility

FS Granted

EXNAM Primary Examiner: Jones, W. Gary; Assistant Examiner: Rees, Dianne

LREP Testa, Hurwitz & Thibault, LLP

CLMN Number of Claims: 47

ECL Exemplary Claim: 1

DRWN 16 Drawing Figure(s); 16 Drawing Page(s)

LN.CNT 1668

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM . . . complete primary structure identification. To date, Edman sequencing and adaptations thereof are the most widely used tools for sequencing certain **protein** and peptides residue by residue, while the enzymatic synthesis method is preferred for sequencing oligonucleotides.

SUMM In the case of **protein** and peptide sequencing, C-terminal sequencing via chemical methods has proven particularly difficult while being only marginally effective, at best. (See, e.g., Spiess, J. (1986)

Methods of **Protein** Characterization: A Practical Handbook (Shively, J. E. ed., Humana Press, N.J.) pp. 363-377; Tsugita et al. (1994) J. **Protein** Chemistry 13:476-479). Consequently, the C-terminus remains a region often not analyzed because of lack of a dependable method.

SUMM . . . . offer a simple approach by which amino acids can be sequentially cleaved residue by residue from the C-terminus of a **protein** or a peptide. Carboxypeptidase Y (CPY), in particular, is an attractive enzyme because it non-specifically cleaves all residues from the . . . .

SUMM . . . . by residue. Not only is this approach labor-intensive, but it is complicated by amino acid contaminants in the enzyme and **protein**/peptide solutions, as well as by enzyme autolysis. A further hindrance to any sequencing effort of this type is the absolute.

SUMM . . . . analysis such as field desorption (Hong et al. (1983) Biomed. Mass Spectrom. 10:450-457), electrospray (Smith et al. (1993) 4 Techniques **Protein** Chem. 463-470), and thermospray (Stachowiak et al. (1988) J. Am. Chem. Soc. 110:1758-1765), it is possible to perform direct mass. . . .

SUMM . . . . digestion of peptides has been combined with other mass spectrometry methods such as plasma desorption (Wang et al. (1992) Techniques **Protein** Chemistry III (ed., R. H. Angeletti; Academic Press, N.Y.) pp. 503-515).

SUMM . . . . obtaining sequence information that incorporates a data interpretation strategy based on integrating mass-to-charge ratio data obtained from a plurality of **parallel mass spectra**.

SUMM The claimed methods are applicable to any polymer, including biopolymers such as DNAs, RNAs, PNAs, **proteins**, peptides and carbohydrates, and modified forms of these polymers. The set of polymer fragments may be created by hydrolysis of. . . .

DETD . . . . moiety. In a currently preferred embodiment, the polymer is a biopolymer selected from, but not limited to, the following group: **proteins**, peptides, DNAs, RNAs, PNAs (peptide nucleic acids), carbohydrates and modified forms thereof.

DETD The claimed invention can be applied to the sequencing of any natural biopolymer such as **proteins**, peptides, nucleic acids, carbohydrates, etc., as well as synthetic biopolymers such as PNA and phosphothiolated nucleic acids. The ladders could. . . .

DETD . . . . collective truncated hydrolyzed polymer fragments. In this manner, for example, sequence information relating to the amino acid sequence of a **protein** can be obtained using carboxypeptidase Y, an agent which acts at the carboxy terminus. By using the methods disclosed herein to generate a series of **protein** hydrolysates related one to the other by consecutive, repetitive liberation of amino acid residues, the skilled artisan can reconstruct the primary sequence of the intact **protein** polymer as described in further detail below.

DETD . . . . invention for this purpose. Thus the above-described subtractive-type sequencing method, through which repetitive removal of successive amino-terminal residues from a **protein** polymer can occur, can also be accomplished with hydrolyzing agents other than enzymes as disclosed herein.

DETD As disclosed herein, this strategy can be applied to the sequencing of any natural biopolymer such as **proteins**, peptides, nucleic acids, carbohydrates, etc. as well as synthetic biopolymers such as PNA and phosphothiolated nucleic acids. The ladders can. . . .

CLM What is claimed is:  
5. The method of claim 4 wherein the biopolymer is selected from the group consisting of DNAs, RNAs, PNAs, **proteins**, peptides, carbohydrates and modified forms thereof.

22. The method of claim 21 wherein the biopolymer is selected from the